1. Consider a particle of mass $m$ subject to a one-dimensional potential of the following form,

$$V(x) = \begin{cases} \frac{1}{2}m\omega^2 x^2, & \text{for } x > 0, \\ \infty, & \text{for } x \leq 0. \end{cases}$$

(a) Determine the possible the bound state energy values of the particle.

The Schrödinger equation for this problem in the interval $0 < x < \infty$ is,

$$\left\{-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2\right\} \psi(x) = E\psi(x).$$

(1)

This is the Schrödinger equation for the one-dimensional harmonic oscillator, whose energy eigenvalues and eigenfunctions are well known. However, in this problem, there is an infinite barrier at $x = 0$, so we must impose an additional boundary condition, $\psi(0) = 0$.

The energy eigenvalues of the one-dimensional harmonic oscillator without the infinite barrier at the origin are $E_n = \hbar\omega(n + \frac{1}{2})$, where $n$ is any non-negative integer. The corresponding energy eigenstates, $\psi_n(x)$, are also eigenstates of parity and satisfy $\psi_n(-x) = (-1)^n\psi_n(x)$. That is, the energy eigenstates are parity even for even $n$ and parity odd for odd $n$. In particular, if $n$ is odd then $\psi_n(0) = 0$. In contrast $\psi_n(x) \neq 0$ for even values of $n$.

We can see this behavior explicitly from the expressions for the harmonic oscillator wave functions. From eq. (B.4.3) of Sakurai and Napolitano,

$$\psi_n(x) = (2^n n!)^{-1/2} \left( \frac{m\omega}{\pi\hbar} \right)^{1/4} \exp \left( -\frac{m\omega x^2}{2\hbar} \right) H_n(x\sqrt{m\omega/\hbar}),$$

(2)

where $H_0(z) = 1$, $H_1(z) = 2z$, ... are the Hermite polynomials. The recursion relation satisfied by the Hermite polynomials, given in eq. (2.5.25) of Sakurai and Napolitano,

$$H_{n+1}(z) = 2zH_n(z) - 2nH_{n-1},$$

can be used to compute $H_n(z)$ for all $n = 2, 3, \ldots$, given $H_0(z) = 1$, $H_1(z) = 2z$. It immediately follows that $H_n(0) = 0$ for odd $n$ and $H_{n+2}(0) = -2(n + 1)H_n(0)$ for even $n$, which yields $H_{2n}(0) = (-2)^n(2n - 1)!! \neq 0$ for all non-negative $n$, after noting that $H_0(0) = 1$.

We conclude that only the odd parity harmonic oscillator wave functions vanish at the origin. These are the allowed square integrable solutions to eq. (1) subject to the boundary condition $\psi(0) = 0$. The corresponding energy eigenvalues are $E_n = \hbar\omega(n + \frac{1}{2})$ for odd positive integers $n$. Writing $n = 2N + 1$, we conclude that the possible bound state energies are

$$E_N = \hbar\omega(2N + \frac{3}{2}), \quad \text{for } N = 0, 1, 2, \ldots.$$
(b) What is the normalized ground state wave function in the coordinate representation?

The ground state wave function for this problem is proportional to the $n = 1$ parity odd energy eigenstate of the one-dimensional harmonic oscillator. Using eq. (2) with $H_1(z) = 2z$,

$$
\psi_{N=0}(x) = \begin{cases} 
Ax \exp\left(-\frac{m\omega x^2}{2\hbar}\right), & \text{for } x > 0, \\
0, & \text{for } x < 0, 
\end{cases}
$$

where $A$ is determined by the normalization condition,

$$
\int_{-\infty}^{\infty} |\psi_{N=0}(x)|^2 dx = 1. \quad (3)
$$

For our problem, due to the fact that $\psi_{N=0}(x) = 0$ for $x < 0$, the square of the normalization constant $A$ must be twice that of the corresponding $n = 1$ harmonic oscillator wave function in order to satisfy eq. (3), i.e., $|A|^2 = 2|A_{HO}|^2$. Since eq. (2) implies that (for $n = 1$),

$$
A_{HO} = \left(\frac{4}{\pi}\right)^{1/4} \left(\frac{m\omega}{\hbar}\right)^{3/4},
$$

it follows that normalized ground state wave function for our problem is,

$$
\psi_{N=0}(x) = \begin{cases} 
\left(\frac{16}{\pi}\right)^{1/4} \left(\frac{m\omega}{\hbar}\right)^{3/4} x \exp\left(-\frac{m\omega x^2}{2\hbar}\right), & \text{for } x > 0, \\
0, & \text{for } x < 0. 
\end{cases}
$$

after setting the overall phase (by convention) to unity. One can verify explicitly that this result satisfies eq. (3).

2. Consider a one-dimensional problem with a Hamiltonian,

$$
H = \frac{P^2}{2m} + V(X), \quad (4)
$$

where $X$ is the position operator and $P$ is the momentum operator. Assume that the spectrum of the Hamiltonian is discrete. Denote the normalized energy eigenstates by $|n\rangle$, and the corresponding energy eigenvalues by $E_n$.

(a) Show that the matrix elements of $X$ and $P$, with respect to a basis consisting of orthonormal energy eigenstates, satisfy the following relation,

$$
\langle k | P | n \rangle = c(k, n) \langle k | X | n \rangle, \quad (5)
$$

where $c(k, n)$ depends on $E_k$ and $E_n$. Determine an explicit expression for $c(k, n)$. 

2
We begin by considering the commutator $[H, X]$, where $H$ is given by eq. (4). Using the canonical commutation relation, $[X, P] = i\hbar I$, and noting that $X$ commutes with any function of $X$, it follows that

$$[H, X] = \left[ \frac{P^2}{2m}, X \right] = \frac{P}{2m} [P, X] + [P, X] \frac{P}{2m} = -\frac{i\hbar}{m} P,$$

after employing the commutator identity, $[AB, C] = A[B, C] + [A, C]B$. Hence, it follows that

$$P = \frac{im}{\hbar} [H, X].$$

Inserting this result into $\langle k | P | n \rangle$ yields,

$$\langle k | P | n \rangle = \frac{im}{\hbar} \langle k | [H, X] | n \rangle = \frac{im}{\hbar} \langle k | (HX - XH) | n \rangle = \frac{im}{\hbar} (E_k - E_n) \langle k | X | n \rangle,$$

where we have used the fact that $|k\rangle$ and $|n\rangle$ are energy eigenstates, e.g., $H |n\rangle = E_n |n\rangle$. Comparing with eq. (5), we conclude that

$$c(k, n) = \frac{im}{\hbar} (E_k - E_n).$$

(b) Evaluate the infinite sum,

$$S \equiv \frac{m}{\hbar^2} \sum_k (E_k - E_n) \left| \langle k | X | n \rangle \right|^2,$$

where the sum is taken over the complete set of energy eigenstates, $|k\rangle$. Show that the sum is equal to a dimensionless constant and determine its value.

Note that the equation $H |n\rangle = E_n |n\rangle$ implies that the energy eigenstates $|n\rangle$ are dimensionless. Moreover, $X$ has the same dimensional units as $\hbar/P$ (cf. the canonical commutation relations). Hence, it follows that $S$ is dimensionless since $P^2/m$ has the dimensions of energy.

It is convenient to introduce the following shorthand notation,

$$\hbar \omega_{kn} \equiv E_k - E_n, \quad X_{kn} \equiv \langle k | X | n \rangle.$$

Then, the result of part (a) can be rewritten as,

$$\langle k | P | n \rangle = i\hbar \omega_{kn} X_{kn}.$$

Since $X$ is a self-adjoint operator, it follows that $X_{kn}^* = X_{nk}$. Hence, eq. (7) can be written as,

$$S = \frac{m}{\hbar} \sum_k \omega_{kn} X_{kn} X_{nk}.$$

Noting that $\omega_{kn} = -\omega_{nk}$, we can rewrite eq. (9) as,

$$S = \frac{m}{2\hbar} \sum_k (\omega_{kn} - \omega_{nk}) X_{kn} X_{nk}.$$
We now can use eqs. (8) and (10) to obtain,

\[ S = -\frac{i}{2\hbar} \left( \sum_k X_{nk} \langle k | P | n \rangle - \sum_k \langle n | P | k \rangle X_{kn} \right). \]  

(11)

Inserting the definitions of \( X_{nk} \) and \( X_{kn} \) in eq. (11) and employing the completeness relation, \( \sum_k |k \rangle \langle k| = I \) (where \( I \) is the identity operator), it follows that

\[ S = -\frac{i}{2\hbar} \left( \sum_k \langle n | X | k \rangle \langle k | P | n \rangle - \sum_k \langle n | P | k \rangle \langle k | X | n \rangle \right) \]

\[ = -\frac{i}{2\hbar} \langle n | (XP - PX) | n \rangle = \frac{1}{2}, \]

after using \([X,P] = i\hbar I\) and \(\langle n|n \rangle = 1\) (since the energy eigenstates are normalized to unity).

**REMARK:**

The identity,

\[ \frac{2m}{\hbar^2} \sum_k (E_k - E_n) |\langle k | X | n \rangle|^2 = 1, \]  

(12)

is called the Thomas-Reiche-Kuhn sum rule, and it plays an important role in quantum radiation theory. It is mentioned on p. 368 of Sakurai and Napolitano, where another method of derivation is proposed. Sakurai and Napolitano suggest considering,

\[ \langle n | [X,[X,H]] | n \rangle = \frac{i\hbar}{m} \langle n | [X,P] | n \rangle = -\frac{\hbar^2}{m} \langle n | n \rangle = -\frac{\hbar^2}{m}, \]  

(13)

after making use of eq. (6) and \([X,P] = i\hbar I\). Then after inserting a complete set of states in appropriate places,

\[ \langle n | [X,[X,H]] | n \rangle = \langle n | (X^2H - 2XHX + HX^2) | n \rangle \]

\[ = \sum_k \langle n | X | k \rangle \langle k | XH | n \rangle - 2 \langle n | XH | k \rangle \langle k | X | n \rangle + \langle n |HX | k \rangle \langle k | X | n \rangle \]

\[ = 2 \sum_k (E_n - E_k) |\langle k | X | n \rangle|^2, \]  

(14)

after using \(H \langle k \rangle = E_k \langle k \rangle\) and \(H \langle n \rangle = E_k \langle n \rangle\). Comparing eqs. (13) and (14), we end up with eq. (12).

There are numerous related sum rules that are similar to the Thomas-Reiche-Kuhn sum rule, which can be derived with similar techniques. For more details, see pp. 211–217 of Hans A. Bethe and Roman Jackiw, *Intermediate Quantum Mechanics*, 3rd edition (Westview Press, Boulder, CO, 1997).

(c) Verify your calculation of \(S\) in part (b) in the case of the one-dimensional harmonic oscillator. That is, assuming \(V(X) = \frac{1}{2}m\omega^2X^2\), compute explicitly \(\langle k | X | n \rangle\) and then use the energy eigenvalues of the one-dimensional harmonic oscillator to explicitly evaluate \(S\).
Using eq. (2.3.25a) of Sakurai and Napolitano,

\[ \langle k | X | n \rangle = \sqrt{\frac{\hbar^2}{2m\omega}} \left[ \sqrt{n} \delta_{k,n-1} + \sqrt{n+1} \delta_{k,n+1} \right]. \]

Thus, for fixed \( n \), the only two non-zero values of \( \langle k | X | n \rangle \) are,

\[ \langle n - 1 | X | n \rangle = \sqrt{\frac{\hbar n}{2m\omega}}, \quad \langle n + 1 | X | n \rangle = \sqrt{\frac{\hbar(n+1)}{2m\omega}}. \]  
\[ (15) \]

Note that if \( n = 0 \), only the second matrix element above is relevant.

The energy eigenvalues of the one-dimensional harmonic oscillator are \( E_n = \hbar \omega (n + \frac{1}{2}) \). Hence, it follows that

\[ E_{n-1} - E_n = -\hbar \omega, \quad E_{n+1} - E_n = \hbar \omega. \]  
\[ (16) \]

Once again, if \( n = 0 \), only the second energy difference above is relevant.

Employing eqs. (15) and (16) in evaluating the sum \( S \) [eq. (7)], only two terms in the sum survive if \( n \neq 0 \),

\[ S = \frac{m}{\hbar^2} \left( \frac{\hbar}{2m\omega} \right) \hbar \omega \left[ -n + (n+1) \right] = \frac{1}{2}. \]

If \( n = 0 \), we replace \(-n + (n+1)\) with 1 since only one term contributes to the sum. The end result is the same, and we again confirm that \( S = \frac{1}{2} \).

3. One would perhaps conclude from the lack of angular momentum in the ground state of the hydrogen atom that the electron is stationary.

(a) To show that this is not so, calculate the probability that the electron’s momentum, if measured, would be found to lie in a momentum element \( d^3p \) centered at momentum \( \vec{p} \).

The wave function for the ground state of hydrogen is

\[ \psi(r, \theta, \phi) = \frac{1}{\sqrt{\pi}} \theta^{-3/2} e^{-r/a_0}, \]

where \( a_0 \equiv \hbar^2/(\mu e^2) \) is the Bohr radius and \( \mu \) is the reduced mass. To compute the probability that the electron has momentum between \( \vec{p} \) and \( \vec{p} + d^3p \), we need to compute the momentum space wave function,

\[ \phi(p) = \frac{1}{(2\pi \hbar)^{3/2}} \int d^3x e^{-ip\cdot\vec{x}/\hbar} \psi(\vec{x}). \]

To perform the above integral, we shall make use of spherical coordinates and choose the z-axis to lie along \( \vec{p} \). Then, \( \vec{p} \cdot \vec{x} = pr \cos \theta \), where \( r \equiv |\vec{x}| \). Hence,

\[ \phi(p) = \frac{1}{(2\pi \hbar)^{3/2}} \left( \frac{1}{\pi a_0^3} \right)^{1/2} \int r^2 dr d\cos \theta d\phi e^{-ipr \cos \theta/\hbar} e^{-r/a_0} \]
\[ = \frac{1}{(2\pi \hbar)^{3/2}} \left( \frac{1}{\pi a_0^3} \right)^{1/2} 2\pi \int_0^\infty r^2 e^{-r/a_0} dr \int_{-1}^1 d\cos \theta e^{-ipr \cos \theta/\hbar} \]
\[ = \frac{1}{(2\pi^2 \hbar^3 a_0^3)^{1/2}} \left( \frac{2\hbar}{p} \right) \int_0^\infty r e^{-r/a_0} \sin \left( \frac{pr}{\hbar} \right) dr. \]  
\[ (17) \]
To evaluate the remaining integral, consider the following function,

\[ F(a) = \int_0^{\infty} e^{-ay} \sin(my) dy , \]

where \( a > 0 \) (the latter is needed for the integral to be convergent). Then,

\[ F(a) = \text{Im} \int_0^{\infty} e^{-ay} e^{imy} dy = \text{Im} \int_0^{\infty} e^{-(a-im)y} dy = \text{Im} \left( \frac{1}{a-im} \right) = \text{Im} \left( \frac{a+im}{a^2+m^2} \right) = \frac{m}{a^2+m^2} . \]

Taking the derivative of the above equation and multiplying by \(-1\) yields,

\[ -\frac{dF}{da} = \int_0^{\infty} ye^{-ay} \sin(my) dy = \frac{2am}{(a^2+m^2)^2}, \quad \text{for } a > 0 . \]

Applying this result to eq. (17), we end up with

\[ \phi(p) = 8\sqrt{\pi} \left( \frac{a_0}{2\pi\hbar} \right)^{3/2} \frac{1}{\left[ 1 + \left( \frac{a_0p}{\hbar} \right)^2 \right]^2} . \tag{18} \]

Note that \( \phi(\vec{p}) \) depends only on the magnitude \( p \equiv |\vec{p}| \). That is, the momentum space ground state wave function is spherically symmetric (which is also true for its coordinate space wave function).

The probability that the electron lies between \( \vec{p} \) and \( \vec{p} + d^3p \) is given by \( |\phi(\vec{p})|^2 d^3p \).

**REMARK 1**: A useful check of our calculation is to verify that the momentum space wave function is normalized to unity (this is a consequence of Parseval’s theorem of Fourier analysis).

\[ \int d^3p |\phi(\vec{p})|^2 = 4\pi \int_0^{\infty} p^2 dp |\phi(\vec{p})|^2 = 256\pi^2 \left( \frac{a_0}{2\pi\hbar} \right)^3 \int_0^{\infty} \frac{p^2 dp}{\left[ 1 + \left( \frac{a_0p}{\hbar} \right)^2 \right]^4} . \]

The integral is recognized as a Beta function,\(^1\)

\[ B(p, q) = \frac{\Gamma(p)\Gamma(q)}{\Gamma(p+q)} = \int_0^{\infty} \frac{u^{p-1} du}{(1+u)^{p+q}} . \]

After a change of variables, \( u = x^2 \), it then follows that

\[ \int_0^{\infty} \frac{x^p dx}{(1+x^2)^r} = \frac{\Gamma\left( \frac{1}{2} \right) \Gamma\left( r - \frac{1}{2} \right) \Gamma(p+1)}{2\Gamma(r)} . \tag{19} \]

Recall that \( \Gamma(n) = (n-1)! \) for positive integer \( n \), \( \Gamma\left( \frac{1}{2} \right) = \sqrt{\pi} \) and \( \Gamma(x+1) = x\Gamma(x) \). It follows that

\[ \int_0^{\infty} \frac{x^2 dx}{(1+x^2)^3} = \frac{\pi}{32} . \]

One then readily verifies that

\[ \int d^3p |\phi(\vec{p})|^2 = 1 . \]

---

REMARK 2: The following alternative derivation of eq. (17) is especially noteworthy, since this method is quite useful in a number of applications. We begin with

\[ \phi(\vec{p}) = \frac{1}{(2\pi\hbar)^{3/2}} \frac{1}{(\pi a_0^3)^{1/2}} \int_0^\infty r^2 e^{-r/a_0} dr \int d\Omega e^{-i\vec{k} \cdot \vec{x}}, \]

(20)

where \( \vec{k} \equiv \vec{p}/\hbar \). Using the expansion of the plane wave in terms of spherical waves,\(^2\)

\[ e^{i\vec{k} \cdot \vec{x}} = 4\pi \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^\ell i^\ell Y_{\ell m}(\hat{r}) Y^*_{\ell m}(\hat{k}) j_\ell(kr), \]

where \( \hat{r} \equiv \vec{x}/r \) (with \( r \equiv |\vec{x}| \)). Integrating over the solid angle \( \Omega = (\theta, \phi) \), where \( \theta \) and \( \phi \) are the polar and azimuthal angles of \( \hat{r} \) with respect to a fixed \( z \) axis,

\[ \int d\Omega e^{i\vec{k} \cdot \vec{x}} = 4\pi \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^\ell i^\ell Y_{\ell m}(\hat{k}) j_\ell(kr) \int d\Omega Y_{\ell m}(\hat{r}), \]

(21)

Recall that the spherical harmonics satisfy the orthonormality relation,

\[ \int d\Omega Y_{\ell m}(\hat{r}) Y^*_{\ell' m'}(\hat{r}) = \delta_{\ell\ell'} \delta_{mm'}. \]

Using the fact that \( Y_{00}(\hat{r}) = (4\pi)^{-1/2} \), it follows that

\[ \int d\Omega Y_{\ell m}(\hat{r}) = \sqrt{4\pi} \delta_{\ell0} \delta_{m0}. \]

Using this result in eq. (21), it follows that

\[ \int d\Omega e^{i\vec{k} \cdot \vec{x}} = 4\pi j_0(kr) = \frac{4\pi \sin(kr)}{kr}. \]

(22)

Taking the complex conjugate of eq. (22) and inserting this result into eq. (20) (with \( k = p/\hbar \)) yields

\[ \phi(\vec{p}) = \frac{1}{(2\pi\hbar^3 a_0^3)^{1/2}} \frac{2\hbar}{p} \int_0^\infty r e^{-r/a_0} \sin \left( \frac{pr}{\hbar} \right) dr, \]

which confirms the result of eq. (17).

(b) What are the electron's mean kinetic and potential energy?

To compute the mean kinetic energy, it is convenient to perform the calculation in momentum space. Thus,

\[ \left\langle \frac{\vec{p}^2}{2\mu} \right\rangle = \int \frac{\vec{p}^2}{2\mu} |\phi(\vec{p})|^2 d^3p = \frac{2\pi}{\mu} \int_0^\infty p^4 dp |\phi(\vec{p})|^2 = \frac{128\pi^2}{\mu} \left( \frac{a_0}{2\pi\hbar} \right)^3 \int_0^\infty \frac{p^4 dp}{\left[ 1 + \left( \frac{a_0p}{\hbar} \right)^2 \right]^4}. \]

Employing the result of eq. (19), we end up with,

\[ \left\langle \frac{\vec{p}^2}{2\mu} \right\rangle = \frac{\hbar^2}{2\mu a_0^2}. \]

(23)

\(^2\)See the class handout entitled, Expansion of plane waves in spherical harmonics.
Next, we turn to the computation of the mean potential energy. The potential energy of the hydrogen atom is

\[ V(r) = -\frac{e^2}{r}. \]

Hence, the mean potential energy is

\[ \langle V(r) \rangle = -e^2 \langle \frac{1}{r} \rangle. \]

It is straightforward to compute

\[ \langle \frac{1}{r} \rangle = \int |\psi(\vec{x})|^2 \frac{1}{r} \, d^3x = 4\pi \frac{1}{\pi a_0^3} \int_0^{\infty} r e^{-2r/a_0} \, dr = \frac{1}{a_0}, \]

after making use of the well known integral

\[ \int_0^{\infty} x^{n-1}e^{-ax} \, dx = \frac{\Gamma(n)}{a^n}, \quad (24) \]

under the assumption that \( a > 0 \). For positive integer \( n \), \( \Gamma(n) = (n-1)! \).

Hence, it follows that

\[ \langle V(r) \rangle = -\frac{e^2}{a_0} = -\frac{\hbar^2}{\mu a_0^2}, \]

where we have replaced \( e^2 = \frac{\hbar^2}{(\mu a_0)} \) using the definition of the Bohr radius, \( a_0 \). Comparing with eq. (23), we obtain

\[ \langle \vec{p}^2/2\mu \rangle = -\frac{1}{2} \langle V(r) \rangle. \quad (25) \]

**REMARK 3:** An alternative calculation of the mean kinetic energy

One can also compute the mean kinetic energy by evaluating the expectation value in position space,

\[ \langle \vec{p}^2/2\mu \rangle = \int \psi^*(\vec{x}) \left( \frac{\hbar^2}{2\mu} \vec{\nabla}^2 \psi(\vec{x}) \right) d^3x. \]

Note that in an \( \ell = 0 \) state, \( \psi(\vec{x}) \) depends only on the radial coordinate \( r \equiv |\vec{x}| \). Hence,

\[ \vec{\nabla}^2 \psi(\vec{x}) = \left( \frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} - \frac{\vec{L}^2}{r^2} \right) \psi(r) = \left( \frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} \right) \psi(r) \]

since \( \vec{L}^2 \) is a purely angular differential operator. Hence,

\[ \langle \vec{p}^2/2\mu \rangle = 4\pi \left( -\frac{\hbar^2}{2\mu} \right) \frac{1}{\pi a_0^3} \int_0^{\infty} \left[ \left( \frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \right) e^{-r/a_0} \right] r^2 e^{-r/a_0} \, dr \]

\[ = 4\pi \left( -\frac{\hbar^2}{2\mu} \right) \frac{1}{\pi a_0^3} \int_0^{\infty} \left( \frac{1}{a_0^2} - \frac{2}{r a_0} \right) r^2 e^{-r/a_0} \, dr = \frac{\hbar^2}{2\mu a_0^2}, \]

after employing eq. (24).
(c) Show that the results of part (b) are consistent with the Virial Theorem.

Using the results of problem 4 of Problem Set 2, the quantum Virial Theorem is,

$$\left\langle \frac{\vec{P}^2}{\mu} \right\rangle = \left\langle \vec{X} \cdot \nabla V \right\rangle.$$  \hspace{1cm} (26)

For a spherically symmetric potential,

$$\vec{X} \cdot \nabla V = r \frac{dV}{dr}.$$  \hspace{1cm} (27)

In particular, for the Coulomb potential, \( V(r) = -\frac{e^2}{r} \),

$$r \frac{dV}{dr} = -V.$$  \hspace{1cm} (28)

Hence, the eq. (26) yields

$$\left\langle \frac{\vec{P}^2}{2\mu} \right\rangle = -\frac{1}{2} \left\langle V(r) \right\rangle,$$  \hspace{1cm} (29)

which confirms the result of eq. (25) obtained above.

4. Consider the Hamiltonian for a free particle of mass \( \mu \) that is confined to a two dimensional cylindrical surface embedded in three dimensions. The cylinder is infinite in extent with a radius \( R \) centered around a symmetry axis that coincides with the \( z \)-axis. The Hamiltonian for this problem is the sum of a kinetic energy term and a rotational kinetic energy term,

$$H = \frac{P_z^2}{2\mu} + \frac{L_z^2}{2\mu R^2},$$  \hspace{1cm} (30)

where \( P_z \) and \( L_z \) are the \( z \)-components of the momentum and angular momentum operators, respectively.

(a) The Hamiltonian given by eq. (30) is invariant under which (continuous) symmetries? Identify the complete set of mutually commuting observables for this problem.

A particle confined to the surface of a infinite cylinder centered around the \( z \)-axis possesses two symmetries: (i) translations in the \( z \) direction; and (ii) rotations about the \( z \)-axis. Translations in the \( z \) direction are generated by \( P_z \) and rotations about the \( z \) axis are generated by \( L_z \). Thus, we expect that

$$[H, P_z] = [H, L_z] = 0.$$  \hspace{1cm} (31)

Indeed, eq. (31) is a consequence of the commutation relations,

$$[P_i, L_j] = i\hbar \epsilon_{ijk} P_k.$$  \hspace{1cm} (32)
Eq. (30) is just the statement that $\vec{P}$ is a vector operator. Moreover, eq. (30) implies that $[P_z, L_z] = 0$. It follows that

$$[H, P_z] = \left[ \frac{P_z^2}{2\mu} + L_z^2, P_z \right] = \frac{1}{2\mu R^2} \left( L_z^2, P_z \right) = \frac{1}{2\mu R^2} \left( L_z [L_z, P_z] + [L_z, P_z] L_z \right) = 0.$$  

Likewise,

$$[H, L_z] = \left[ \frac{P_z^2}{2\mu} + \frac{L_z^2}{2\mu R^2}, L_z \right] = \frac{1}{2\mu} \left( P_z^2, L_z \right) = \frac{1}{2\mu} \left( P_z [P_z, L_z] + [P_z, L_z] P_z \right) = 0.$$  

On the other hand, a similar computation implies that $[H, P_x] \neq 0$, $[H, P_y] \neq 0$, $[H, L_x] \neq 0$ and $[H, L_y] \neq 0$, where we have again made use of eq. (30). It therefore follows that the complete set of mutually commuting observables for this problem consists of the three operators, $H$, $P_z$ and $L_z$.

(b) Employing cylindrical coordinates $(\rho, \phi, z)$, where $x = \rho \cos \phi$ and $y = \rho \sin \phi$, the surface of the cylinder corresponds to $\rho = R$. Hence, the Hamiltonian of eq. (28) describes an effective two dimensional problem with coordinates $z$ and $\phi$. Write down the time-independent Schrödinger equation in the coordinate representation for this problem, and determine the allowed energy eigenvalues and the corresponding eigenfunctions of the Hamiltonian $H$.

In the coordinate representation,

$$\langle \vec{x} | \vec{P} | \psi \rangle = -i\hbar \vec{\nabla} \psi(\vec{x}), \quad \langle \vec{x} | \vec{L} | \psi \rangle = -i\hbar \vec{x} \times \vec{\nabla} \psi(\vec{x}).$$

Employing cylindrical coordinates,

$$\langle \rho, \phi, z | P_z | \psi \rangle = -i\hbar \frac{\partial \psi}{\partial z}, \quad \langle \rho, \phi, z | L_z | \psi \rangle = -i\hbar \frac{\partial \psi}{\partial \phi}. \quad (31)$$

Note that the operator representation of $L_z$ is the same as in two dimensions with polar coordinates. Indeed, in class, I showed that for $x = \rho \cos \phi$ and $y = \rho \sin \phi$,

$$\frac{\partial}{\partial \phi} = \frac{\partial x}{\partial \phi} \frac{\partial}{\partial x} + \frac{\partial y}{\partial \phi} \frac{\partial}{\partial y} = -y \frac{\partial}{\partial \phi} + x \frac{\partial}{\partial y} = (\vec{x} \times \vec{\nabla})_z.$$  

Moreover, the fact that $\rho = R$ is fixed does not alter the results quoted in eq. (31).

Hence, starting from eq. (28), the time-independent Schrödinger equation in the coordinate representation is given by

$$-\frac{\hbar^2}{2\mu} \left( \frac{\partial^2}{\partial z^2} + \frac{1}{R^2} \frac{\partial^2}{\partial \phi^2} \right) \psi(z, \phi) = E \psi(z, \phi). \quad (32)$$

One can solve this equation using the separation of variables technique. Equivalently, in light of $[H, L_z] = 0$, one can choose $\psi(z, \phi)$ to be a simultaneous eigenstate of $H$ and $L_z$. This means that one can replace $L_z^2$ in eq. (28) with its eigenvalue, $m^2 \hbar^2$, where $m$ is any integer. Hence,

$$\psi(z, \phi) = Z(z)e^{im\phi}, \quad (33)$$

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where we are using the same eigenfunctions of $L_z$ that were obtained in class when we examined spherically symmetric two-dimensional problems using polar coordinates.

Inserting eq. (33) into eq. (32), we obtain an ordinary differential equation for $Z(z)$,

$$\frac{\hbar^2}{2\mu} \left( \frac{d^2}{dz^2} - \frac{m^2}{R^2} \right) Z(z) = E Z(z). \quad (34)$$

Writing $E = \hbar^2 k^2 / (2\mu)$, eq. (34) yields

$$\left( \frac{d^2}{dz^2} + k^2 - \frac{m^2}{R^2} \right) Z(z) = 0. \quad (35)$$

We consider two cases. First, if $k^2 < m^2 / R^2$, then the solution to eq. (35) is

$$Z(z) = A \exp \left\{ z \left( \frac{m^2}{R^2} - k^2 \right)^{1/2} \right\} + B \exp \left\{ -z \left( \frac{m^2}{R^2} - k^2 \right)^{1/2} \right\},$$

where $A$ and $B$ are constants. But, this solution is not acceptable since it is exponentially growing either as $z \to \infty$ if $B = 0$ or as $z \to -\infty$ if $A = 0$.

Second, if $k^2 > m^2 / R^2$, then the solution to eq. (35) is

$$Z(z) = A \exp \left\{ iz \left( k^2 - \frac{m^2}{R^2} \right)^{1/2} \right\} + B \exp \left\{ -iz \left( k^2 - \frac{m^2}{R^2} \right)^{1/2} \right\},$$

where $A$ and $B$ are constants. This solution corresponds to plane waves propagating in the positive and negative $z$ directions, as one would expect for a free particle.

Thus, we have found that the possible energy eigenvalues are any non-negative value that satisfies,

$$E = \frac{\hbar^2 k^2}{2\mu} \geq \frac{\hbar^2 m^2}{2\mu R^2},$$

for any integer value of $m$, with the corresponding eigenfunction,

$$\psi(z, \phi) = e^{im\phi} \left[ A \exp \left\{ iz \left( \frac{2\mu E}{\hbar^2} - \frac{m^2}{R^2} \right)^{1/2} \right\} + B \exp \left\{ -iz \left( \frac{2\mu E}{\hbar^2} - \frac{m^2}{R^2} \right)^{1/2} \right\} \right].$$